

**2018 SPRING TECHNICAL MEETING  
EASTERN STATES SECTIONS OF THE COMBUSTION INSTITUTE  
The Pennsylvania State University, Pennsylvania  
March 4-7, 2018**

**Sunday, March 4, 2018**

**17:00 – 20:00 Days Inn Foyer: Registration**

**13:00 – 16:00 108 Sackett Building: Cantera Workshop**

**15:30 – 17:30 Days Inn: ESSCI Executive Board Meeting**

**18:00 – 20:00 Days Inn Foyer: Welcome Reception**

**Monday, March 5, 2018**

**7:00 – 18:00 Days Inn Foyer: Registration**

**8:15 Main Hall: Welcome Remarks/Announcements**

**Jacqueline O'Connor, The Pennsylvania State University**

**Yuan Xuan, The Pennsylvania State University**

**8:30 Main Hall:**

**Plenary Lecture: William H. Green, Massachusetts Institute of Technology**

**Title: *Predicting Combustion Chemistry & Focusing on the Important Aspects***

**Session Chair: Yuan Xuan, The Pennsylvania State University**

**9:30 – 9:45 Transition to Morning Session**

	<b>Reaction Kinetics I Room 1 Session Chair: M.P Burke</b>	<b>Oxygenates Room 2 Session Chair: F.M. Haas</b>	<b>Droplets Room 3 Session Chair: S.G. Tuttle</b>
<b>9:45</b>	<b>1A01: Evaluated rate constants for <i>i</i>-butane + H and CH<sub>3</sub>: Shock tube experiments with Bayesian model optimization</b> <i>L.A. Mertens, I.A. Awan, J.A. Manion</i> <i>National Institute of Standards and Technology</i>	<b>1B01: Shock tube studies of methyl propanoate and methane kinetics</b> <i>S. Jouzdani, D.M. Coomb, X. Zheng, B. Akhi-Kumgeh</i> <i>Syracuse University</i>	<b>1C01: Three stage quasi-steady droplet burning behavior of <i>n</i>-alkane droplets at elevated pressure conditions: Hot, warm and cool flame combustion</b> <i>T. Farouk<sup>1</sup>, D. Dietrich<sup>2</sup>, F.L. Dryer<sup>1,3</sup></i> <sup>1</sup> <i>University of South Carolina</i> <sup>2</sup> <i>NASA Glenn Research Center</i> <sup>3</sup> <i>Princeton University</i>

	<b>Reaction Kinetics I</b> <b>Room 1</b> <b>Session Chair: M.P. Burke</b>	<b>Oxygenates</b> <b>Room 2</b> <b>Session Chair: F.M. Haas</b>	<b>Droplets</b> <b>Room 3</b> <b>Session Chair: S.G. Tuttle</b>
<b>10:00</b>	<b>1A02: Kinetics of H atom addition to cyclopentane</b> <i>J.A. Manion, I.A. Awan</i> <i>National Institute of Standards and Technology</i>	<b>1B02: Shock tube and CO laser-absorption measurements during cyclopentanone oxidation</b> <i>E. Ninnemann<sup>1</sup>, S. Barak<sup>1</sup>, O. Pryor<sup>1</sup>, W.H. Green<sup>2</sup>, K. Zhang<sup>3</sup>, W.J. Pitz<sup>3</sup>, S. Vasu<sup>1</sup></i> <sup>1</sup> <i>University of Central Florida</i> <sup>2</sup> <i>Massachusetts Institute of Technology</i> <sup>3</sup> <i>Lawrence Livermore National Laboratory</i>	<b>1C02: Computational study of oscillatory cool flame dynamics for submillimeter sized n-heptane droplet</b> <i>F.E. Alam<sup>1</sup>, A.C. Aghdam<sup>1</sup>, F.L. Dryer<sup>1,2</sup>, T.I. Farouk<sup>1</sup></i> <sup>1</sup> <i>University of South Carolina</i> <sup>2</sup> <i>Princeton University</i>
<b>10:15</b>	<b>1A03: Intramolecular phenyl migration in hexylbenzene radicals: An ab initio/TST study</b> <i>S. Khanniche, W.H. Green</i> <i>Massachusetts Institute of Technology</i>	<b>1B03: Premixed flame propagation in mixtures of cyclopentanone/air</b> <i>G. Kim, B. Almansour, R. Blair, K. Ahmed, J. Kapat, S.S. Vasu</i> <i>University of Central Florida</i>	<b>1C03: Motion of a merged drop upon impacting a liquid pool</b> <i>A. Saha<sup>1</sup>, Y. Wei<sup>1,2</sup>, X. Tang<sup>1</sup>, C.K. Law<sup>1</sup></i> <sup>1</sup> <i>Princeton University</i> <sup>2</sup> <i>Xi'an Jiaotong University</i>
<b>10:30 – 11:00</b>	<b>BREAK – Days Inn Foyer</b>		
	<b>Reaction Kinetics II</b> <b>Room 1</b> <b>Session Chair: C.B. Reuter</b>	<b>Sooting Tendencies</b> <b>Room 2</b> <b>Session Chair: S.H. Won</b>	<b>Spray Flames</b> <b>Room 3</b> <b>Session Chair: J.H. MacArt</b>
<b>11:00</b>	<b>1A04: A fully-automated kinetic mechanism lumping algorithm</b> <i>L. Backer, P. Pepiot</i> <i>Cornell University</i>	<b>1B04: Sooting tendencies of aromatic hydrocarbons with oxygencontaining side-chains</b> <i>B.P. Beekley<sup>1</sup>, C.S. McEnally<sup>1</sup>, P.C. St. John<sup>2</sup>, S. Kim<sup>2</sup>, A. Jain<sup>3</sup>, H. Kwon<sup>3</sup>, Y. Xuan<sup>3</sup>, L.D. Pfefferle<sup>1</sup></i> <sup>1</sup> <i>Yale University</i> <sup>2</sup> <i>National Renewable Energy Laboratory</i> <sup>3</sup> <i>The Pennsylvania State University</i>	<b>1C04: Droplet size and velocity measurements in a heptane/propane spray flame</b> <i>B.T. Fisher, S.G. Tuttle, A.D. Tuesta</i> <i>Naval Research Laboratory</i>
<b>11:15</b>	<b>1A05: Introducing a workflow for improving kinetic models: Case study using butanol</b> <i>S.K. Sirumalla<sup>1</sup>, M.A. Mayer<sup>2</sup>, K.E. Niemeyer<sup>2</sup>, R.H. West<sup>1</sup></i> <sup>1</sup> <i>Northeastern University</i> <sup>2</sup> <i>Oregon State University</i>	<b>1B05: Numerical investigation of pressure dependence of yield sooting tendencies</b> <i>Y. Xuan<sup>1</sup>, C.S. McEnally<sup>2</sup>, A. Jain<sup>1</sup>, H. Kwon<sup>1</sup>, L.D. Pfefferle<sup>2</sup></i> <sup>1</sup> <i>The Pennsylvania State University</i> <sup>2</sup> <i>Yale University</i>	<b>1C05: Droplet flamelet-generated manifold modeling for two-phase turbulent combustion</b> <i>B.T. Bojko, P.E. DesJardin</i> <i>University at Buffalo, State University of New York</i>
<b>11:30</b>	<b>1A06: An analytical jacobian generator for reduced chemical kinetic models involving quasi-steady-state assumptions</b> <i>P. Sharma, H. Goyal, P. Pepiot</i> <i>Cornell University</i>	<b>1B06: Sensitivity analysis and uncertainty propagation in numerical simulations of yield sooting tendencies</b> <i>Y. Xuan, K. Mohhan, A. Jain, H. Kwon</i> <i>The Pennsylvania State University</i>	<b>1C06: Reynolds-averaged Navier-Stokes simulations of a piloted heptane/propane spray flame</b> <i>D.A. Kessler, B.T. Fisher, A.D. Tuesta, S.G. Tuttle</i> <i>Naval Research Laboratory</i>

	<b>Reaction Kinetics II</b> <b>Room 1</b> <b>Session Chair: C.B. Reuter</b>	<b>Sooting Tendencies</b> <b>Room 2</b> <b>Session Chair: S.H. Won</b>	<b>Spray Flames</b> <b>Room 3</b> <b>Session Chair: J.H. MacArt</b>
11:45	<b>1A07: ChemKED for profile-resolved data: A discussion of some salient data standard features</b> <i>F.M. Haas<sup>1</sup>, C.F. Goldsmith<sup>2</sup>, M.P. Burke<sup>3</sup>, B.W. Weber<sup>4</sup>, K.E. Niemeyer<sup>5</sup></i> <sup>1</sup> Rowan University <sup>2</sup> Brown University <sup>3</sup> Columbia University <sup>4</sup> University of Connecticut <sup>5</sup> Oregon State University	<b>1B07: Analyzing the robustness of the yield sooting index as a measure of sooting tendency</b> <i>M.J. Montgomery, D.D. Das, C.S. McEnally, L.D. Pfefferle</i> Yale University	<b>1C07: A numerical investigation of the chemical kinetics in the low temperature oxidation process of n-heptane spray (I)</b> <i>Y. Li<sup>1</sup>, H. Ge<sup>2</sup>, H. Li<sup>1</sup></i> <sup>1</sup> West Virginia University <sup>2</sup> Texas Tech University
12:00 – 13:30	<b>Lunch</b> <b>Graduate Student Workshop – Room 4</b>		
13:30 – 14:30	<b>Main Hall – Glassman Lecture</b> <b>Invited Speaker: Wenting Sun, Georgia Tech</b> <b>Title: <i>The Effect of Ozone Addition on Combustion: What We Know and What We Don't</i></b> <b>Session Chair: Paul Papas, UTRC</b>		
	<b>2:30 – 2:45 Transition to Afternoon Sessions</b>		
	<b>Reaction Kinetics III</b> <b>Room 1</b> <b>Session Chair: M.E. Fuller</b>	<b>Sooting Flame Simulations</b> <b>Room 2</b> <b>Session Chair: T. Grenga</b>	<b>New Devices</b> <b>Room 3</b> <b>Session Chair: H. Goyal</b>
14:45	<b>1A08: Shock tube and kinetic modelling study of organo phosphorus compounds used as chemical weapon simulants</b> <i>S. Neupane, F. Barnes, S. Barak, E. Ninnemann, Z. Loparo, A.E. Masunov, S.S. Vasu</i> University of Central Florida	<b>1B08: A multi-moment sectional method to predict the soot size distribution</b> <i>S. Yang, M.E. Mueller</i> Princeton University	<b>1C08: A “scale-up” Swiss-roll combustor and its application in waste gas incineration</b> <i>J. Crawmer<sup>1</sup>, C.-H. Chen<sup>1</sup>, B. Richard<sup>1</sup>, H. Pearlman<sup>1</sup>, P. Ronney<sup>2</sup>, T. Edwards<sup>3</sup></i> <sup>1</sup> Advanced Cooling Technologies, Inc. <sup>2</sup> The University of Southern California <sup>3</sup> Temple University
15:00	<b>1A09: Carbon addition lowers initiation and iodine release temperatures from iodine oxide-based biocidal energetic materials</b> <i>T. Wu, X. Wang, S. Holdren, M.R. Zachariah</i> University of Maryland	<b>1B09: Subfilter transport modeling for large eddy simulation of turbulent nonpremixed sooting flames</b> <i>S. Yang, J.K. Lew, M.E. Mueller</i> Princeton University	<b>1C09: Swiss-roll JP-8 fuel reformer with direct center fuel injection and mixing chamber design</b> <i>J. Crawmer<sup>1</sup>, C.-H. Chen<sup>1</sup>, B. Richard<sup>1</sup>, H. Pearlman<sup>1</sup>, P. Ronney<sup>2</sup></i> <sup>1</sup> Advanced Cooling Technologies, Inc. <sup>2</sup> The University of Southern California

	<b>Reaction Kinetics III Room 1 Session Chair: M.E. Fuller</b>	<b>Sooting Flame Simulations Room 2 Session Chair: T. Grenga</b>	<b>New Devices Room 3 Session Chair: H. Goyal</b>
<b>15:15</b>	<b>1A10: Thermochemistry and kinetic analysis on the reactions and mechanisms of CH<sub>3</sub>SCH<sub>2</sub>CH<sub>3</sub> with oxygen and OH radicals</b> <i>G. Song, J.W. Bozzelli New Jersey Institute of Technology</i>	<b>1B10: Simulations of soot formation in high-pressure transient spray flames</b> <i>S. Ferreyro Fernandez, D.C. Haworth The Pennsylvania State University</i>	<b>1C10: Microwave plasma processing of methane: Optical diagnostics and carbon characterizations</b> <i>R. Vander Wal<sup>1</sup>, A. Sengupta<sup>1</sup>, E. Musselman<sup>2</sup>, K. Zeller<sup>2</sup>, G. Skoptsov<sup>2</sup> <sup>1</sup>The Pennsylvania State University <sup>2</sup>H Quest Vanguard, Inc.</i>
<b>15:30</b>	<b>1A11: Ion-molecule reactions relevant to the detection of atmospheric oxidized mercury by chemical ionization mass spectrometry</b> <i>F.J. Guzman, M. Cooper, J. Antley, J. Bozzelli, A. Khalizov New Jersey Institute of Technology</i>	<b>1B11: Large eddy simulations of staged pressurized oxy-combustion</b> <i>F.N. Karaismail<sup>1</sup>, A. Gopan<sup>2</sup>, R.L. Axelbaum<sup>2</sup>, I. Celik<sup>1</sup>, B.M. Kumfer<sup>2</sup> <sup>1</sup>West Virginia University <sup>2</sup>Washington University in St. Louis</i>	<b>1C11: Development of a constant volume combustion chamber for material synthesis</b> <i>M. Morovatiyan, M. Shahsavan, J.H. Mack University of Massachusetts, Lowell</i>
<b>15:45 – 16:00</b>	<b>BREAK – Days Inn Foyer</b>		
	<b>Laminar Flames Room 1 Session Chair: V. Acharya</b>	<b>Soot Room 2 Session Chair: S. Yang</b>	<b>Coal and Biomass Room 3 Session Chair: X. Zhao</b>
<b>16:00</b>	<b>1A12: Double luminous zones in inverse laminar jet diffusion flames</b> <i>Z. Wang<sup>1</sup>, P.B. Sunderland<sup>1</sup>, R.L. Axelbaum<sup>2</sup> <sup>1</sup>University of Maryland <sup>2</sup>Washington University in St. Louis</i>	<b>1B12: Reconciliation of carbon oxidation rates and activation energies based on changing nanostructure</b> <i>M. Singh<sup>1</sup>, C.K. Gaddam<sup>1</sup>, R.L. Vander Wal<sup>1</sup>, X. Chen<sup>2</sup>, A. Yezerets<sup>2</sup>, K. Kamasamudram<sup>2</sup> <sup>1</sup>The Pennsylvania State University <sup>2</sup>Cummins, Inc.</i>	<b>1C12: Nitrogen oxide evolution in oxy-coal combustion</b> <i>S.K. Sirumalla, A. Panahi, A. Purohit, A. Baugher, Y.A. Levendis, R.H. West Northeastern University</i>
<b>16:15</b>	<b>1A13: Low-temperature multistage diffusion flames</b> <i>O.R. Yehia, C.B. Reuter, Y. Ju Princeton University</i>	<b>1B13: Analysis of East Asian soot-based inksticks through Raman spectroscopy</b> <i>J. Giaccari<sup>1,2</sup>, J.H. Miller<sup>1</sup> <sup>1</sup>George Washington University <sup>2</sup>Smithsonian Institution</i>	<b>1C13: Effect of variability in biomass properties on biomass devolatilization</b> <i>H. Goyal, P. Pepiot Cornell University</i>
<b>16:30</b>	<b>1A14: Multi-modal counterflow flames under autoignitive conditions</b> <i>T. Grenga, J.F. MacArt, M.E. Mueller Princeton University</i>	<b>1B14: Informing TiRe-LII assumptions of soot nanostructure and optical properties for estimation of soot primary particle diameter</b> <i>M. Singh, R.L. Vander Wal The Pennsylvania State University</i>	<b>1C14: A study on pulverized coal ignition using a two-stage flat-flame burner with a transition from a reducing to oxidizing environment</b> <i>A. Adeosun, D. Khatri, A. Gopan, Z. Yang, T. Li, R.L. Axelbaum Washington University in St. Louis</i>

	<b>Laminar Flames Room 1 Session Chair: V. Acharya</b>	<b>Soot Room 2 Session Chair: S. Yang</b>	<b>Coal and Biomass Room 3 Session Chair: X. Zhao</b>
<b>16:45</b>	<b>1A15: Transient interactions between a premixed double flame and a vortex</b> <i>C.B. Reuter<sup>1</sup>, V.R. Katta<sup>2</sup>, O.R. Yehia<sup>1</sup>, Y. Ju<sup>1</sup></i> <sup>1</sup> Princeton University <sup>2</sup> Innovative Scientific Solutions, Inc.	<b>1B15: Soot derivatization for source identification</b> <i>M. Singh, R.L. Vander Wal</i> The Pennsylvania State University	<b>1C15: Explosive dust characteristics evaluation of pulverized Pittsburgh coal using ASTM E1226-12a</b> <i>J. Miller, P. Mulligan, C. Johnson</i> Missouri University of Science and Technology
<b>17:00</b>	<b>1A16: Laminar flame propagation in supercritical hydrogen/air and methane/air mixtures</b> <i>W. Liang, W. Li, C.K. Law</i> Princeton University	<b>1B16: The effects of oxygenated fuels on soot particle nanostructure</b> <i>J. Zhu, C.S. McEnally, L.D. Pfefferle</i> Yale University	<b>1C16: Coal particle ignition in a combustion environment with a reducing-to-oxidizing transition</b> <i>D. Khatri, A. Adeosun, A. Gopan, Z. Wang, R.L. Axelbaum</i> Washington University in St. Louis
<b>17:15</b>	<b>1A17: Various regimes of premixed flame propagation in obstructed channels with both extremes open</b> <i>A. Adebisi<sup>1</sup>, E. Ridgeway<sup>1</sup>, R. Alkandari<sup>1</sup>, A. Cathreno<sup>1</sup>, D. Valiev<sup>2</sup>, V. Akkerman<sup>1</sup></i> <sup>1</sup> West Virginia University <sup>2</sup> Tsinghua University	<b>1B17: Effects of hydrogen addition on the structure of <i>n</i>-dodecane laminar, co-flow flame</b> <i>A. Makwana, M. Linevsky, S. Iyer, R. Santoro, T. Litzinger, J. O'Connor</i> The Pennsylvania State University	<b>1C17: Predicting particle deposition for flow over a circular cylinder in combustion environments</b> <i>A. Gopan, Z. Yang, R.L. Axelbaum</i> Washington University in St. Louis
<b>17:30</b>	<b>1A18: Computational simulations of nonequidiffusive premixed flames in obstructed pipes</b> <i>A. Adebisi<sup>1</sup>, G. Idowu<sup>1</sup>, D. Valiev<sup>2</sup>, V. Akkerman<sup>1</sup></i> <sup>1</sup> West Virginia University <sup>2</sup> Tsinghua University	<b>1B18: Soot characteristics of light naphtha in a constant volume combustion chamber using two-color pyrometry</b> <i>Z. Wu<sup>1</sup>, L. Wang<sup>1</sup>, J.A. Badra<sup>2</sup>, W.L. Roberts<sup>3</sup>, T. Fang<sup>1</sup></i> <sup>1</sup> North Carolina State University <sup>2</sup> Saudi Aramco <sup>3</sup> King Abdullah University of Science and Technology	<b>1C18: Spectroscopic emission measurements and system level modeling of a two-stage wood-fired hydronic heater: Effects of non-homogeneous fuel decomposition</b> <i>J.M. Weisberger, J.P. Richter, J.C. Mollendorf, P.E. DesJardin</i> University at Buffalo, the State University of New York
<b>17:45</b>	<b>1A19: Transient ellipsoidal flames in microgravity</b> <i>A. Markan<sup>1</sup>, H.R. Baum<sup>1</sup>, P.B. Sunderland<sup>1</sup>, J.G. Quintiere<sup>1</sup>, J.L. de Ris<sup>2</sup></i> <sup>1</sup> University of Maryland <sup>2</sup> FM Global, retired	<b>1B19: Quantification of nanostructure changes by HRTEM and fringe analyses during NO<sub>2</sub>-O<sub>2</sub> oxidation</b> <i>M. Srilomsak<sup>1,2</sup>, M. Singh<sup>2</sup>, K. Hanamura<sup>1</sup>, R.L. Vander Wal<sup>2</sup></i> <sup>1</sup> Tokyo Institute of Technology <sup>2</sup> The Pennsylvania State University	<b>1C19: Experimental investigation of the stabilization and structure of turbulent cool diffusion flames</b> <i>C.B. Reuter<sup>1</sup>, O.R. Yehia<sup>1</sup>, S.H. Won<sup>2</sup>, M.K. Fu<sup>1</sup>, K. Kokmanian<sup>1</sup>, M. Hultmark<sup>1</sup>, Y. Ju<sup>1</sup></i> <sup>1</sup> Princeton University <sup>2</sup> University of South Carolina
<b>19:00 Young Faculty Mixer –Federal Taphouse</b>			

**Tuesday, March 6, 2018**

**8:00 – 16:00**      **Days Inn Foyer: Registration**

**8:15**                      **Main Hall: Announcements**  
**Jacqueline O'Connor, The Pennsylvania State University**  
**Yuan Xuan, The Pennsylvania State University**

**8:30**                      **Main Hall:**  
**Plenary Lecture: Harsha K. Chelliah, University of Virginia**  
**Title: *Hypersonic Propulsion: Challenges in Thermal Management and Flame Stabilization over a Range of Flow Conditions***  
**Session Chair: Daniel C. Haworth, The Pennsylvania State University**

**9:30 – 9:45 Transition to Morning Session**

	<b>Reaction Kinetics IV Room 1 Session Chair: G. Song</b>	<b>Fire - Instrumentation Room 2 Session Chair: A. Gopan</b>	<b>Turbulent Flames Room 3 Session Chair: C.E. Dumitrescu</b>
<b>9:45</b>	<b>2A01: A study of JP-10 pyrolysis by molecular beam mass spectrometry with comparison to literature model</b> <i>G.P. Simms, H.K. Chelliah</i> <i>University of Virginia</i>	<b>2B01: CMOS based high-speed camera pyrometry measurements for validation of upward flame spread modeling</b> <i>S.S. Aphale, P.E. DesJardin</i> <i>University at Buffalo, State University of New York</i>	<b>2C01: The effect of non-axisymmetric fuel staging on flame structure in a multiple-nozzle model turbine combustor</b> <i>O. Sekulich, W. Culler, J. O'Connor</i> <i>The Pennsylvania State University</i>
<b>10:00</b>	<b>2A02: Investigation of ethylene ozonolysis reaction's temporal behavior and products using plug flow reactor</b> <i>B. Wu, X. Gao, W. Sun</i> <i>Georgia Institute of Technology</i>	<b>2B02: Designing a gas sampling system for a 3 MW fire calorimeter using an experimental approach</b> <i>J. Hashempour, R. Ranellone, A. Simeoni, N. Dembsey</i> <i>Worcester Polytechnic Institute</i>	<b>2C02: The influence of mixedness on ignition for hydrogen direct injection in a constant volume combustion chamber</b> <i>M. Shahsavan, M. Morovatiyan, J.H. Mack</i> <i>University of Massachusetts Lowell</i>
<b>10:15</b>	<b>2A03: Catalytic ignition and pressure dependence of methane/air combustion over palladium oxide</b> <i>R. Sui<sup>1,2</sup>, W. Liang<sup>1</sup>, J. Mantzaras<sup>2</sup>, C.K. Law<sup>1</sup></i> <sup>1</sup> <i>Princeton University</i> <sup>2</sup> <i>Paul Scherrer Institute</i>	<b>2B03: Flight test demonstration of LED-based fire sensors for space propulsion vehicles</b> <i>A.C. Terracciano<sup>1</sup>, K. Thurmond<sup>1</sup>, M. Villar<sup>1</sup>, J. Urso<sup>1</sup>, E. Ninnemann<sup>1</sup>, A. Parupalli<sup>1</sup>, Z. Loparo<sup>1</sup>, N. Demidovich<sup>2</sup>, J.S. Kapat<sup>1</sup>, S.S. Vasu<sup>1</sup></i> <sup>1</sup> <i>University of Central Florida</i> <sup>2</sup> <i>FAA Office of Commercial Space Transportation</i>	<b>2C03: The effects of piloting on turbulent flame structure</b> <i>R. Shupp<sup>1</sup>, A. Tyagi<sup>1</sup>, I. Boxx<sup>2</sup>, S. Peluso<sup>1</sup>, J. O'Connor<sup>1</sup></i> <sup>1</sup> <i>The Pennsylvania State University</i> <sup>2</sup> <i>DLR, German Aerospace Center</i>
<b>10:30 – 11:00</b>	<b>BREAK – Days Inn Foyer</b>		

	<b>Reaction Kinetics V</b> <b>Room 1</b> <b>Session Chair: T.I. Farouk</b>	<b>Pool Fires</b> <b>Room 2</b> <b>Session Chair: B.T. Fisher</b>	<b>Turbulent Combustion Modeling</b> <b>Room 3</b> <b>Session Chair: L. Backer</b>
<b>11:00</b>	<b>2A04: Impact of cyclo-alkanes on ignition propensity measured as derived cetane number in multi-component mixtures</b> <i>D. Carpenter, S. Nates, S.J. Lim, F.L. Dryer, S.H. Won</i> <i>University of South Carolina</i>	<b>2B04: In situ burn ignition testing methods and results for California crude oils</b> <i>S.G. Tuttle, B.T. Fisher, C.J. Pfitzner, T.N. Loegel, K.M. Hinnant</i> <i>U.S. Naval Research Laboratory</i>	<b>2C04: Challenges for large eddy simulation of partially premixed turbulent combustion using reduced-order manifold flame structure models</b> <i>B.A. Perry, M.E. Mueller</i> <i>Princeton University</i>
<b>11:15</b>	<b>2A05: Surrogate formation based on chemical functional group analysis</b> <i>S. Nates, D. Carpenter, S.J. Lim, F. Dryer, S.H. Won</i> <i>University of South Carolina</i>	<b>2B05: Evaluating foam degradation and fuel transport rates through novel surfactant firefighting foams for the purpose of AFFF perfluorocarbon replacement</b> <i>K. Hinnant, A. Snow, S. Giles, R. Ananth</i> <i>U.S. Naval Research Laboratory</i>	<b>2C05: Topologically conditioned chemical pathways for turbulent lean premixed n-dodecane/air flames</b> <i>D. Dasgupta<sup>1</sup>, W. Sun<sup>1</sup>, M. Day<sup>2</sup>, A.J. Aspden<sup>3</sup>, T. Lieuwen<sup>1</sup></i> <i><sup>1</sup>Georgia Institute of Technology</i> <i><sup>2</sup>Lawrence Berkeley National Laboratory</i> <i><sup>3</sup>Newcastle University</i>
<b>11:30</b>	<b>2A06: Pyrolysis of fuel mixtures at supercritical conditions: A ReaxFF molecular dynamics study</b> <i>S. Shabnam, C. Ashraf, A. Jain, Y. Xuan, A.C.T. van Duin</i> <i>The Pennsylvania State University</i>	<b>2B06: Effect of low temperature wall on the extinction and fuel layer distribution of pool fires</b> <i>C. Li<sup>1</sup>, H.F. Farahani<sup>1</sup>, R. Yang<sup>2</sup>, A.S. Rangwala<sup>1</sup></i> <i><sup>1</sup>Worcester Polytechnic Institute</i> <i><sup>2</sup>Tsinghua University</i>	<b>2C06: On the accessed region of composition space in turbulent diffusion flames</b> <i>A.S. Newale, Y. Liang, S.B. Pope, P. Pepiot</i> <i>Cornell University</i>
<b>11:45</b>	<b>2A07: Fuel distillation affects spray flame blowout thresholds</b> <i>J.A. Lefkowitz, F.M. Haas</i> <i>Rowan University</i>	<b>2B07: Liquid-pool fire extinction characteristics of aqueous foams generated from fluorine-free surfactants</b> <i>R. Ananth, S. Giles, K. Hinnant, X. Zhuang, A. Snow, J. Fleming, J. Farley</i> <i>U.S. Naval Research Laboratory</i>	<b>2C07: A comprehensive model for non-adiabatic multi-modal combustion using physically-derived reduced-order manifolds</b> <i>A.C. Nunno, M.E. Mueller</i> <i>Princeton University</i>
<b>12:00 – 13:15</b>	<b>Lunch</b> <b>Diversity Workshop – Room 4</b>		
	<b>13:15 – 13:30 Transition to Afternoon Sessions</b>		

	<b>Reaction Kinetics VI Room 1 Session Chair: S. Khanniche</b>	<b>Solid Propellants and Explosives Room 2 Session Chair: S.S. Vasu</b>	<b>Turbulent Flames Room 3 Session Chair: J.W. Meadows</b>
<b>13:30</b>	<p><b>2A08: Addressing discrepancies in hydrogen abstraction by OOH radical via automatic transition state theory calculations</b>  <i>N. Harms, R.H. West  Northeastern University</i></p>	<p><b>2B08: Mechanism development of aqueous hydroxylammonium nitrate under thermal decomposition conditions</b>  <i>K. Zhang, S.T. Thynell  The Pennsylvania State University</i></p>	<p><b>2C08: DNS of cavity stabilized premixed turbulent flame with a high-order immersed boundary method</b>  <i>A.H. Rauch<sup>1</sup>, K. Aditya<sup>2</sup>, H. Kolla<sup>2</sup>, J.H. Chen<sup>2</sup>,  H.K. Chelliah<sup>1</sup>  <sup>1</sup>University of Virginia  <sup>2</sup>Sandia National Laboratories</i></p>
<b>13:45</b>	<p><b>2A09: Multiscale informatics of reactions involved in H<sub>2</sub>O<sub>2</sub> decomposition in the presence of dopants</b>  <i>C.E. LaGrotta, M.C. Barbet, L. Lei, M.P. Burke  Columbia University</i></p>	<p><b>2B09: Development of gas-phase reaction mechanism for ammonium perchlorate using quantum mechanics calculations</b>  <i>T. Chatterjee, S.T. Thynell  The Pennsylvania State University</i></p>	<p><b>2C09: Large eddy simulation and probability density function modelling of swirling Cambridge/Sandia turbulent stratified flame series</b>  <i>H. Turkeri, X. Zhao  University of Connecticut</i></p>
<b>14:00</b>	<p><b>2A10: Studies of pentane oxidation and pyrolysis in nanosecond-pulsed plasma discharges using in-situ laser diagnostics</b>  <i>A. Rousso<sup>1</sup>, X. Mao<sup>1,2</sup>, Q. Chen<sup>2</sup>, Y. Ju<sup>1</sup>  <sup>1</sup>Princeton University  <sup>2</sup>Beijing Jiaotong University</i></p>	<p><b>2B10: Investigation into the structure-function relation of 3D printed energetic films: Single layer formulation study</b>  <i>M.C. Rehwoldt, H. Wang, N. Eckman, D. Kline,  M.R. Zachariah  University of Maryland</i></p>	<p><b>2C10: Budgets of flame-conditioned second-order turbulence statistics in low and high Karlovitz number turbulent premixed jet flames</b>  <i>J.F. MacArt, T. Grenga, M.E. Mueller  Princeton University</i></p>
<b>14:15</b>	<p><b>2A11: Low-temperature oxidation of n-dodecane in a microflow tube reactor: Temperature and residence times effects</b>  <i>K. Dang, H.K. Chelliah  University of Virginia</i></p>	<p><b>2B11: Liquid-phase decomposition of RDX: Formation of oxy-s-triazine and 1,3,4-oxadiazole</b>  <i>L. Patidar, M. Khichar, S.T. Thynell  The Pennsylvania State University</i></p>	<p><b>2C11: Topology of local flame-flame interaction events in turbulent flames</b>  <i>A. Tyagi<sup>1</sup>, I. Boxx<sup>2</sup>, R. Shupp<sup>1</sup>, S. Peluso<sup>1</sup>, J. O'Connor<sup>1</sup>  <sup>1</sup>The Pennsylvania State University  <sup>2</sup>DLR, German Aerospace Center</i></p>
<b>14:30</b>	<p><b>2A12: Effects of <i>sp</i><sup>2</sup> carbon on low-temperature oxidation of cyclic hydrocarbons</b>  <i>J.C. Davis<sup>1</sup>, A.L. Koritzke<sup>1</sup>, R.L. Caravan<sup>2</sup>,  M.G. Christianson<sup>1</sup>, D.L. Osborn<sup>2</sup>, C.A. Taatjes<sup>2</sup>,  B. Rotavera<sup>1</sup>  <sup>1</sup>University of Georgia  <sup>2</sup>Sandia National Laboratories</i></p>	<p><b>2B12: Computational study of condensed-phase kinetics during combustion of pure RDX</b>  <i>M. Khichar, L. Patidar, S.T. Thynell  The Pennsylvania State University</i></p>	<p><b>2C12: Cellular instability in expanding turbulent flames</b>  <i>Z. Liu, A. Saha, S. Yang, C.K. Law  Princeton University</i></p>
<b>14:45</b>	<p><b>2A13: The kinetic study of excited singlet oxygen atom O(<sup>1</sup>D) reactions with acetylene</b>  <i>C. Yan, C. Teng, T. Chen, A. Rousso, G. Wysocki, Y. Ju  Princeton University</i></p>	<p><b>2B13: Impact of chemically termolecular reactions on the kinetics of energetic materials</b>  <i>R.E. Cornell, C.E. LaGrotta, M.C. Barbet, M.P. Burke  Columbia University</i></p>	<p><b>2C13: Numerical simulations of oxy-fuel premixed combustion in supercritical CO<sub>2</sub>-diluted environment</b>  <i>A. Adebisi<sup>1</sup>, V. Akkerman<sup>1</sup>, K. Kemenov<sup>2</sup>  <sup>1</sup>West Virginia University  <sup>2</sup>Symplectic Research, Inc.</i></p>



15:00 – 15:30				BREAK – Days Inn Foyer			
NOx Kinetics Room 1 Session Chair: N. Harms		Refrigerants Room 2 Session Chair: P.B. Sunderland		Combustion Instabilities Room 3 Session Chair: W. Culler			
15:30	<p><b>2A14: On the relative importance of HONO versus HNO<sub>2</sub> in low-temperature combustion</b>  <i>M.E. Fuller, C.F. Goldsmith</i>  <i>Brown University</i></p>	<p><b>2B14: An improved test method for refrigerant flammability limits in a 12 L vessel</b>  <i>D.K. Kim, A.E. Klieger, P.Q. Lomax, C.G. McCoy, J.Y. Reymann, P.B. Sunderland</i>  <i>University of Maryland</i></p>	<p><b>2C14: Thermoacoustic linear stability model with porous media and mean flow effects</b>  <i>C. Dowd, J. Meadows</i>  <i>Virginia Tech</i></p>				
15:45	<p><b>2A15: A computational investigation into the kinetics of NO + CH<sub>2</sub>CCH and its effect on NO reduction</b>  <i>A.D. Danilack, C.F. Goldsmith</i>  <i>Brown University</i></p>	<p><b>2B15: Deflagrations of mildly flammable refrigerant-air mixtures in closed volumes</b>  <i>K.C. Gottiparthi<sup>1</sup>, P. Papas<sup>1</sup>, V. Sankaran<sup>1</sup>, P. Verma<sup>1</sup>, R. Lord<sup>2</sup>, L. Burns<sup>2</sup></i>  <sup>1</sup><i>United Technologies Research Center</i>  <sup>2</sup><i>Carrier Corporation</i></p>	<p><b>2C15: Thermoacoustic analysis with statistically based flame transfer function extracted from computational fluid dynamics</b>  <i>S. Sampathkumar, J.W. Meadows</i>  <i>Virginia Tech</i></p>				
16:00	<p><b>2A16: Multidimensional numerical investigation of NO<sub>x</sub> formation in a burner coupled flow tube configuration</b>  <i>S.F. Ahmed<sup>1</sup>, A. Dasgupta<sup>2</sup>, F.L. Dryer<sup>1,3</sup>, T.I. Farouk<sup>1</sup></i>  <sup>1</sup><i>University of South Carolina</i>  <sup>2</sup><i>Combustion Science and Engineering Inc.</i>  <sup>3</sup><i>Princeton University</i></p>	<p><b>2B16: Predicted burning velocities of C1 and C2 hydrofluorocarbon refrigerant flames with air</b>  <i>G. Linteris, V. Babushok</i>  <i>National Institute of Standards and Technology</i></p>	<p><b>2C16: Effects of transverse nozzle location on high-frequency transverse combustion instabilities in can combustors</b>  <i>V. Acharya, T. Lieuwen</i>  <i>Georgia Institute of Technology</i></p>				
16:15	<p><b>2A17: Kinetic study of NO<sub>x</sub> formation for synthetic natural gas combustion under gas turbine relevant conditions</b>  <i>F.E. Alam<sup>1</sup>, S.F. Ahmed<sup>1</sup>, F.L. Dryer<sup>1,2</sup>, T.I. Farouk<sup>1</sup></i>  <sup>1</sup><i>University of South Carolina</i>  <sup>2</sup><i>Princeton University</i></p>	<p><b>2B17: Development and validation of a mechanism for flame propagation in R-32/air mixtures</b>  <i>D.R. Burgess, Jr., J.A. Manion, R.R. Burrell, V.I. Babushok, M.J. Hegetschweiler, G.T. Linteris</i>  <i>National Institute of Standards and Technology</i></p>	<p><b>2C17: Effects of the equivalence ratio transient durations on self-excited combustion instability time scales in a single nozzle combustor</b>  <i>X. Chen, W. Culler, S. Peluso, D. Santavicca, J. O'Connor</i>  <i>The Pennsylvania State University</i></p>				
16:30 – 16:45 Short Break							
16:45 – 17:45	<p>ESSCI General Member Meeting  Main Hall  <i>(All Encouraged to Attend)</i></p>						
18:00 – 19:00	<p>Cocktail Hour  Nittany Lion Inn – Boardroom Foyer</p>						
19:00 – 22:00	<p>ESSCI Banquet  Nittany Lion Inn – Boardroom</p>						

Wednesday, March 7, 2018

**8:15**            **Main Hall: Announcements**  
**Jacqueline O'Connor, The Pennsylvania State University**  
**Yuan Xuan, The Pennsylvania State University**

**8:30**            **Main Hall:**  
**Plenary Lecture: Erica Smithwick, The Pennsylvania State University**  
**Title: Firescapes in the mid-Atlantic: Mismatches between social perceptions and prescribed re use**  
**Session Chair: Jacqueline O'Connor, The Pennsylvania State University**

**9:30 – 9:45 Transition to Morning Session**

	<b>Reaction Kinetics VII Room 1 Session Chair: B. Rotavera</b>	<b>Fire - Modeling Room 2 Session Chair: A.S. Newale</b>	<b>SI Engines Room 3 Session Chair: A.C. Nunno</b>
<b>9:45</b>	<b>3A01: Accounting for real-gas effects in high-density combustion chamber</b> <i>C. Zheng, B. Akih-Kumgeh</i> <i>Syracuse University</i>	<b>3B01: Large eddy simulations of a methane-air turbulent line fire using flamelet combustion and non-gray gas radiation models</b> <i>A. Marchand<sup>1</sup>, V.M. Le<sup>1,2</sup>, S. Verma<sup>1</sup>, J. White<sup>1</sup>, A.W. Marshall<sup>1</sup>, T. Rogaume<sup>2</sup>, F. Richard<sup>2</sup>, J. Luche<sup>2</sup>, A. Trouvé<sup>1</sup></i> <sup>1</sup> <i>University of Maryland</i> <sup>2</sup> <i>Université de Poitiers</i>	<b>3C01: Role of low-temperature chemistry in detonation of <i>n</i>-heptane/oxygen/diluent mixtures</b> <i>W. Liang<sup>1</sup>, R. Mével<sup>2</sup>, C.K. Law<sup>1,2</sup></i> <sup>1</sup> <i>Princeton University</i> <sup>2</sup> <i>Tsinghua University</i>
<b>10:00</b>	<b>3A02: Effect of the presence of water molecules on syngas combustion: A ReaxFF molecular dynamics study</b> <i>C. Ashraf, S. Shabnam, A.C.T. van Duin</i> <i>The Pennsylvania State University</i>	<b>3B02: Memory optimization of a radiative heat transfer solver for fire simulations</b> <i>A. Caratenuto, P. Zhang, B. Wu, X. Zhao</i> <i>University of Connecticut</i>	<b>3C02: Effects of thermal and fuel stratifications and turbulence transport on knocking formation for dimethyl ether/air mixtures</b> <i>T. Zhang<sup>1</sup>, W. Sun<sup>1</sup>, L. Wang<sup>2</sup>, Y. Ju<sup>1</sup></i> <sup>1</sup> <i>Princeton University</i> <sup>2</sup> <i>Tsinghua University</i>
<b>10:15</b>	<b>3A03: High-throughput screening for reactive and energy-transferring collider effects in complex-forming reactions</b> <i>M.C. Barbet, K. McCullough, M.P. Burke</i> <i>Columbia University</i>	<b>3B03: Development of 3D pyrolysis in FDS</b> <i>M. Bruns<sup>1</sup>, R. McDermott<sup>1</sup>, S. Benkorichi<sup>2</sup>, S. Hostikka<sup>3</sup></i> <sup>1</sup> <i>National Institute of Standards and Technology</i> <sup>2</sup> <i>Omega Fire Engineering Ltd.</i> <sup>3</sup> <i>Aalto University</i>	<b>3C03: Large-eddy simulations of a spark ignition IC engine</b> <i>S.J. Kazmouz, D.C. Haworth</i> <i>The Pennsylvania State University</i>

**10:30 – 11:00**            **BREAK – Days Inn Foyer**

	<b>Reaction Kinetics VIII</b> <b>Room 1</b> <b>Session Chair: A. Makwana</b>	<b>Fire</b> <b>Room 2</b> <b>Session Chair: A. Marchand</b>	<b>IC Engines</b> <b>Room 3</b> <b>Session Chair: J.H. Mack</b>
11:00	<b>3A04: Dynamic evaluation of multi-component pressure dependence in multi-channel reactions: A case study of CH<sub>3</sub>+OH system</b> <i>L. Lei, M.P. Burke</i> <i>Columbia University</i>	<b>3B04: Critical ignition conditions of structural materials by cylindrical firebrands</b> <i>H. Salehizadeh, R.S.P. Hakes, M.J. Gollner</i> <i>University of Maryland</i>	<b>3C04: Influence of turbulence-radiation interactions in engine radiation heat transfer</b> <i>C. Paul<sup>1</sup>, D.C. Haworth<sup>1</sup>, S. Roy<sup>2</sup>, M.F. Modest<sup>3</sup></i> <i><sup>1</sup>The Pennsylvania State University</i> <i><sup>2</sup>Marquette University</i> <i><sup>3</sup>University of California, Merced</i>
11:15	<b>3A05: Prompt dissociations of propyl radicals from OH + C<sub>3</sub>H<sub>8</sub> and their role in combustion simulations</b> <i>R. Sivaramakrishnan<sup>1</sup>, C.F. Goldsmith<sup>2</sup>, S.L. Peukert<sup>1</sup>, J.V. Michael<sup>1</sup></i> <i><sup>1</sup>Argonne National Laboratory</i> <i><sup>2</sup>Brown University</i>	<b>3B05: Fire dynamics and forensic analysis of compartment fires</b> <i>S.P. Kozhumal, G.E. Gorbett</i> <i>Eastern Kentucky University</i>	<b>3C05: CFD-based non-equilibrium wall heat transfer models for engine-relevant conditions</b> <i>A. Sircar, D.C. Haworth</i> <i>The Pennsylvania State University</i>
11:30	<b>3A06: Explosion limits of H<sub>2</sub>/CH<sub>4</sub>/O<sub>2</sub> mixtures: Analyticity and dominant kinetics</b> <i>W. Liang, Z. Liu, C.K. Law</i> <i>Princeton University</i>	<b>3B06: A study of cavity effect on flame spread over kerosene-soaked sand bed</b> <i>N. Mofidi, A.S. Rangwala</i> <i>Worcester Polytechnic Institute</i>	<b>3C06: Combustion visualization in a single-cylinder heavy-duty CI engine converted to natural gas SI operation</b> <i>J. Liu, C.E. Dumitrescu</i> <i>West Virginia University</i>
11:45	<b>3A07: Measurement of methane autoignition delays in a shock tube under supercritical carbon dioxide conditions</b> <i>M. Karimi, B. Ochs, W. Sun, D. Ranjan</i> <i>Georgia Institute of Technology</i>	<b>3B07: The structure of a turbulent line fire subjected to cross-flow</b> <i>S. Verma, A. Trouvé</i> <i>University of Maryland</i>	<b>3C07: High load diesel engine-generator power improvement with advanced combustion modes</b> <i>M. Walker, D.L. Prak, L. Hamilton, J. Cowart</i> <i>U.S. Naval Academy</i>
12:00	<b>3A08: Color camera pyrometry and its impact in reaction visualization of energetic materials</b> <i>D.J. Kline, R.J. Jacob, P.M. Guerieri, M.R. Zachariah</i> <i>University of Maryland</i>	<b>3B08: Conditions for formation of the blue whirl</b> <i>Y. Hu<sup>1,2</sup>, S.B. Hariharan<sup>2</sup>, M.J. Gollner<sup>2</sup>, E.S. Oran<sup>2</sup></i> <i><sup>1</sup>Tsinghua University</i> <i><sup>2</sup>University of Maryland</i>	<b>3C08: Compression-ignition of GDI sprays in a constant volume combustion chamber</b> <i>L. Wang<sup>1</sup>, F. Wang<sup>1</sup>, W.L. Roberts<sup>2</sup>, T. Fang<sup>1</sup></i> <i><sup>1</sup>North Carolina State University</i> <i><sup>2</sup>King Abdullah University of Science and Technology</i>
12:15		<b>3B09: Effects of ullage on combustion efficiency and plume entrainment of pit fires</b> <i>V. Kimmerly, A.S. Rangwala</i> <i>Worcester Polytechnic Institute</i>	
12:30	<b>Lunch 12:30 – 13:30</b> <b>Adjourn</b> <b>The Pennsylvania State University Combustion Lab Tour</b> <b>Meet at 13:30 at the Atrium of Research East</b>		

**2018 EASTERN STATES SPRING TECHNICAL MEETING AUTHOR LISTING**

<b>AUTHOR</b>	<b>PAPER#</b>	<b>AUTHOR</b>	<b>PAPER#</b>	<b>AUTHOR</b>	<b>PAPER#</b>	<b>AUTHOR</b>	<b>PAPER#</b>
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